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Large-scale parallel lattice Boltzmann–cellular automaton model of two-dimensional dendritic growth☆

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ABSTRACT

An extremely scalable lattice Boltzmann (LB)–cellular automaton (CA) model for simulations of two-dimensional (2D) dendritic solidification under forced convection is presented. The model incorporates effects of phase change, solute diffusion, melt convection, and heat transport. The LB model represents the diffusion, convection, and heat transfer phenomena. The dendrite growth is driven by a difference between actual and equilibrium liquid composition at the solid–liquid interface. The CA technique is deployed to track the new interface cells. The computer program was parallelized using the Message Passing Interface (MPI) technique. Parallel scaling of the algorithm was studied and major scalability bottlenecks were identified. Efficiency loss attributable to the high memory bandwidth requirement of the algorithm was observed when using multiple cores per processor. Parallel writing of the output variables of interest was implemented in the binary Hierarchical Data Format 5 (HDF5) to improve the output performance, and to simplify visualization. Calculations were carried out in single precision arithmetic without significant loss in accuracy, resulting in 50% reduction of memory and computational time requirements. The presented solidification model shows a very good scalability up to centimeter size domains, including more than ten million of dendrites.

Program summary

Program title: 2Ddend
Catalogue identifier: AEQZ_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEQZ_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, UK
Licensing provisions: Standard CPC license, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 29,767
No. of bytes in distributed program, including test data, etc.: 3131,367
Distribution format: tar.gz
Programming language: Fortran 90.
Computer: Linux PC and clusters.
Operating system: Linux.
Has the code been vectorized or parallelized?: Yes. Program is parallelized using MPI. Number of processors used: 1–50,000
RAM: Memory requirements depend on the grid size
Classification: 6.5, 7.7.
External routines: MPI (http://www.mcs.anl.gov/research/projects/mpi/), HDF5 (http://www.hdfgroup.org/HDF5/)

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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Nature of problem:
Dendritic growth in undercooled Al–3 wt% Cu alloy melt under forced convection.

Solution method:
The lattice Boltzmann model solves the diffusion, convection, and heat transfer phenomena. The cellular automaton technique is deployed to track the solid/liquid interface.

Restrictions:
Heat transfer is calculated uncoupled from the fluid flow. Thermal diffusivity is constant.

Unusual features:
Novel technique, utilizing periodic duplication of a pre-grown "incubation" domain, is applied for the scaleup test.

Running time:
Running time varies from minutes to days depending on the domain size and number of computational cores.

1. Introduction

The microstructure and accompanying mechanical properties of the engineering components based on metallic alloys are established primarily in the process of solidification. In this process, the crystalline matrix of the solid material is formed according to the morphology and composition of the crystalline dendrites growing from their nucleation sites in an undercooled melt. Among other processes, solidification occurs during casting and welding, which are commonly deployed in modern manufacturing. Therefore, understanding of the phenomena of solidification is vital to improve the strength and durability of the products that encounter casting or welding in the manufacturing process.

The phenomenon of dendrite growth during solidification has been the subject of numerous studies. When a new simulation technique is developed, the first and necessary step is to validate it by examining the growth of a single dendrite, or a small set of dendrites in a microscale specimen. If the model compares well with physical experiments, it can be deployed for simulating larger domains. Since the new techniques are initially implemented in serial computer codes, the size of the simulation domain is often limited by the memory and computational speed of a single computer. Despite the current advances in large scale parallel supercomputing, only a handful of studies of larger, close-to-physical size solidification domains have been performed. Parallel simulations of the 3D dendrite growth [1] have been performed utilizing the phase field model [2]. Improved, multigrid phase field schemes presented by Guo et al. [3] allow parallel simulations of tens of complex shape 2D dendrites in a simulation domain of up to 25 μm $\times$ 25 μm size. Shimokawabe et al. [4] deployed a modern heterogeneous GPU/CPU architecture to perform the first petascale 3D solidification simulations in a domain size of up to 3.1 mm $\times$ 4.8 mm $\times$ 7.7 mm. However, none of these models included convection.

For the solidification models incorporating effects of convection, the lattice Boltzmann method (LBM) is an attractive alternative to the conventional, finite difference and finite element based fluid dynamics solvers. Among LBM advantages are simple formulation and locality, with locality facilitating parallel implementation.

In this work, the cellular automaton (CA) technique instead of a phase field model is deployed to track the solid–liquid interface, as suggested by Sun et al. [5]. The interface kinetics is driven by the local difference between actual and equilibrium liquid composition [6]. A serial version of the present LBM–CA model with a smaller number of dendrites was validated against theoretical and experimental results [7–11]. In the following, we demonstrate nearly ideal parallel scaling of the model up to millions of dendrites in centimeter size domains, including thermal, convection, and solute redistribution effects.

2. Continuum formulation for fluid flow, solute transport, and heat transfer

Melt flow is assumed to be incompressible, without external force and pressure gradient, governed by simplified Navier–Stokes equations (NSEs)

$$\rho\left[\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right]=\nabla\cdot(\mu\nabla\boldsymbol{u})\,, \tag{1}$$

where $\mu=\nu\rho$ is the dynamic viscosity of the melt.

The time evolution of the solute concentration in the presence of fluid flow is given by the convection–diffusion equation

$$\frac{\partial C_{\mathrm{l}}}{\partial t}+\boldsymbol{u}\cdot\nabla C_{\mathrm{l}}=\nabla\cdot(D_{\mathrm{l}}\nabla C_{\mathrm{l}})\,, \tag{2}$$

where C_{l} is the solute concentration in the liquid phase and D_{l} is the diffusion coefficient of solute in the liquid phase. Solute diffusion in the solid phase is neglected.

Heat transfer in the presence of fluid flow is also governed by a convection–diffusion type (2) equation

$$\frac{\partial T}{\partial t}+\boldsymbol{u}\cdot\nabla T=\nabla\cdot(\alpha\nabla T)\,, \tag{3}$$

where T is the temperature, t is time, and α is the thermal diffusivity.

3. Lattice Boltzmann method

The lattice Boltzmann method (LBM) [12–15] is a simulation technique for solving fluid flow and transport equations. LBM treats the fluid as a set of fictitious particles located on a d-dimensional lattice. Primary variables of LBM are particle distribution functions f_i. Particle distribution functions represent portions of a local particle density moving in the directions of discrete velocities. For a lattice representation DdQz, each point in the d-dimensional lattice links to neighboring points with z links that correspond to velocity directions. We chose the D2Q9 lattice, utilizing nine velocity vectors $\boldsymbol{e}_0$–$\boldsymbol{e}_8$ in two dimensions, as shown in Fig. 1. Distribution functions f_0–f_8 correspond to velocity vectors $\boldsymbol{e}_0$–$\boldsymbol{e}_8$. Using the collision model of Bhatnagar–Gross–Krook (BGK) [16] with a single relaxation time, the evolution of distribution functions is given by

$$f_i(\boldsymbol{r}+\boldsymbol{e}_i\Delta t,t+\Delta t)=f_i(\boldsymbol{r},t)+\frac{1}{\tau_{\mathrm{u}}}\left(f_i^{\mathrm{eq}}(\boldsymbol{r},t)-f_i(\boldsymbol{r},t)\right) \tag{4}$$